



# STIC Search Report

EIC 1700

STIC Database Tracking Number: 112822

**TO:** Dawn Garrett  
**Location:** REM 5C 75  
**Art Unit :** 1774  
**January 30, 2004**

**Case Serial Number:** 10/644872

**From:** Barba Koroma  
**Location:** EIC 1700  
REM EO4 A30  
**Phone:** 571 272 2546

**barba.koroma@uspto.gov**

## Search Notes

Examiner Garrett,  
Please find attached results of the search you requested. Various components of the claimed invention as spelt out in the claims were searched in REGISTRY and CAPLUS databases. For your convenience, titles of hits have been listed to help you peruse the results set quickly. This is followed by a detailed printout of records. Please let me know if you have any questions.

Thanks.

Page 1Garrett10644872

=> file reg  
FILE 'REGISTRY' ENTERED AT 11:15:12 ON 30 JAN 2004  
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STRUCTURE FILE UPDATES: 28 JAN 2004 HIGHEST RN 642928-00-5  
DICTIONARY FILE UPDATES: 28 JAN 2004 HIGHEST RN 642928-00-5

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
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to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> file caplus  
FILE 'CAPLUS' ENTERED AT 11:15:17 ON 30 JAN 2004  
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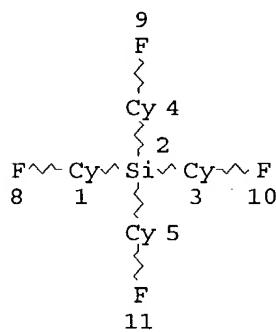
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FILE COVERS 1907 - 30 Jan 2004 VOL 140 ISS 6  
FILE LAST UPDATED: 29 Jan 2004 (20040129/ED)

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

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L57 STR

KOROMA EIC1700



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L58 ( 6) SEA FILE=REGISTRY SSS FUL L57  
L59       20 SEA FILE=CAPLUS ABB=ON PLU=ON L58

=> d ti 1-20

L59 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Intramolecular interactions in aromatic compounds: V. Electronic structure  
of polyfluoroaromatic silanes and related hydrocarbons

L59 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Olefin polymerization and process therefor

L59 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Substituent effect on electronegativity of Ar<sub>3</sub>Si and Ar<sub>3</sub>Sn groups:  
comparison of the results of ab initio quantum-chemical calculations with  
<sup>19</sup>F NMR data for Ar<sub>3</sub>MQC<sub>6</sub>H<sub>4</sub>F-4 compounds

L59 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI A convenient preparation of pentafluorophenyl(fluoro)silanes: reactivity  
of pentafluorophenyltrifluorosilane

L59 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Thermodynamic simulation of deposition of molybdenum and tungsten  
disilicides in metalorganic CVD processes

L59 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Photoelectron helium spectra of the pentafluorophenyl derivatives of Group  
IV and V elements

L59 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Reactions of arylmethysilanes and tetraarylsilanes with xenon difluoride in the presence of fluoride ions

L59 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Pentafluorophenyliodine(V) compounds, part 1. Preparation of pentafluorophenyliodine tetrafluoride and other aryliodine tetrafluorides by reaction of iodine pentafluoride with arylsilanes

L59 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI The crystal structure of tetrakis(pentafluorophenyl)silane

L59 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI A fluorine-19 NMR investigation of the transmission of electronic effects in triaryl(4-fluorophenyl)silanes

L59 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI NMR studies of pentafluorophenyl-substituted silanes. I. Relations between chemical shifts, coupling constants, and  $(p-d)\pi$  interactions

L59 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Fragmentation and rearrangement processes in the mass spectra of perhalogenoaromatic compounds. II. Pentafluorophenyl derivatives of group IV

L59 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI A direct preparation of some pentafluorophenyl-containing silanes

L59 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI The fluorine-19 NMR spectra of some pentafluorophenyl compounds of group IV elements

L59 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Polyhalo-organometallic and -organometalloidal compounds. VIII. Preparation of some pentafluorophenyl substituted organosilicon compounds

L59 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Pentafiuorophenyl organometallic compounds of group IV elements

L59 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Tetrakis(pentafluorophenyl)silane

L59 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Pentafluoroiodobenzene

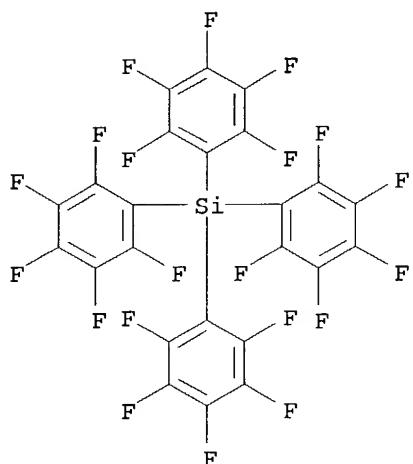
L59 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Synthesis of organosilicon compounds, particularly those containing halophenyl groups

L59 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Preparation and thermal stability of tetrakis(pentafluorophenyl)silane and

tris(pentafluorophenyl)phosphine

=> d ibib abs hitstr ind total

L59 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2000:525583 CAPLUS  
DOCUMENT NUMBER: 133:252494  
TITLE: Intramolecular interactions in aromatic compounds: V.  
Electronic structure of polyfluoroaromatic silanes and  
related hydrocarbons  
AUTHOR(S): Krupoder, S. A.; Okotrub, A. V.; Villem, N. V.;  
Villem, J. J.; Furin, G. G.; Salakhutdinov, N. F.;  
Poleshchuk, O. Kh.  
CORPORATE SOURCE: Institute of Organic Chemistry, Siberian Branch,  
Russian Academy of Sciences, Novosibirsk, Russia  
SOURCE: Russian Journal of General Chemistry (Translation of  
Zhurnal Obshchei Khimii) (2000), 70(1), 101-110  
CODEN: RJGCEK; ISSN: 1070-3632  
PUBLISHER: MAIK Nauka/Interperiodica Publishing  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The electronic structure of pentafluorophenyl-substituted silanes  
ArnSiMe4-n (Ar = C6H5, C6F5, 4-FC6H4, 2,3,5,6-F4C5N; n = 1; Ar = C6H5,  
C6F5, n = 2, 4) was studied by x-ray emission and He(I) photoelectron  
spectroscopy. The He(I) photoelectron spectra were measured and  
interpreted from MNDO calcns., anal. of the p-fluoro effect, and relative  
intensities. Substitution of C6F5 for C6H5 in aryltrimethyl- and  
diaryldimethylsilanes results in enhanced  $\pi$  interaction between the  
aryl and SiMen groups (n = 2, 3) by higher  $\pi$  levels and has almost no  
effect on the charge on the Si atom.  
IT 1524-78-3, Tetrakis(pentafluorophenyl)silane  
RL: PRP (Properties)  
(electronic structure determined by photoelectron spectra, x-ray emission  
and MNDO calcns.)  
RN 1524-78-3 CAPLUS  
CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

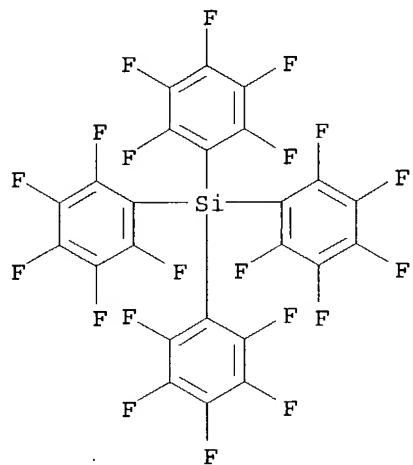


CC 29-6 (Organometallic and Organometalloidal Compounds)  
Section cross-reference(s): 22  
ST electronic structure silane phenyl fluorophenyl MNDO; photoelectron spectrum silane phenyl fluorophenyl; x ray emission silane phenyl fluorophenyl; fluorine substituent effect photoelectron spectrum fluorophenylosilane  
IT Electronic structure  
MNDO (molecular orbital)  
Photoelectron spectra  
X-ray emission  
(of Ph and polyfluoroarom. silanes)  
IT Substituent effects  
(of fluorine in polyfluoroarom. silanes on photoelectron spectra)  
IT Ionization potential  
(of polyfluoroarom. silanes)  
IT Silanes  
RL: PRP (Properties)  
(polyfluoroarom.; electronic structure determined by photoelectron spectra,  
x-ray emission and MNDO calcns.)  
IT 455-17-4, 4-Fluorophenyl(trimethyl)silane 768-32-1,  
Trimethyl(phenyl)silane 778-24-5, Dimethyl(diphenyl)silane 1048-08-4,  
Tetraphenylosilane 1206-46-8, Pentafluorophenyl(trimethyl)silane  
1524-78-3, Tetrakis(pentafluorophenyl)silane 10536-62-6  
16297-29-3  
RL: PRP (Properties)  
(electronic structure determined by photoelectron spectra, x-ray emission  
and MNDO calcns.)  
IT 75-76-3, Tetramethylsilane  
RL: PRP (Properties)  
(model compound; electronic structure determined by photoelectron spectra,  
x-ray emission and MNDO calcns.)  
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L59 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1998:490675 CAPLUS  
 DOCUMENT NUMBER: 129:149360  
 TITLE: Olefin polymerization and process therefor  
 INVENTOR(S): Van Tol, Maurits Frederik Hendrik  
 PATENT ASSIGNEE(S): DSM N.V., Neth.; Van Tol, Maurits Frederik Hendrik  
 SOURCE: PCT Int. Appl., 21 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.   | KIND | DATE     | APPLICATION NO. | DATE       |
|--|------|----------|-----------------|------------|
| WO 9830603   | A1   | 19980716 | WO 1997-NL696   | 19971215   |
| W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS,<br>JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO,<br>SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ,<br>MD, RU, TJ, TM |      |          |                 |            |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI,<br>FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM,<br>GA, GN, ML, MR, NE, SN, TD, TG   |      |          |                 |            |
| NL 1004991   | C2   | 19980715 | NL 1997-1004991 | 19970114   |
| AU 9853475   | A1   | 19980803 | AU 1998-53475   | 19971215   |
| EP 954540  | A1   | 19991110 | EP 1997-950491  | 19971215   |
| R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE, PT, FI  |      |          |                 |            |
| CN 1248979   | A    | 20000329 | CN 1997-182023  | 19971215   |
| JP 2002514247  | T2   | 20020514 | JP 1998-530771  | 19971215   |
| US 6218487   | B1   | 20010417 | US 1999-352842  | 19990713   |
| PRIORITY APPLN. INFO.:   |      |          | NL 1997-1004991 | A 19970114 |
|  |      |          | US 1997-38160P  | P 19970213 |
|  |      |          | WO 1997-NL696   | W 19971215 |

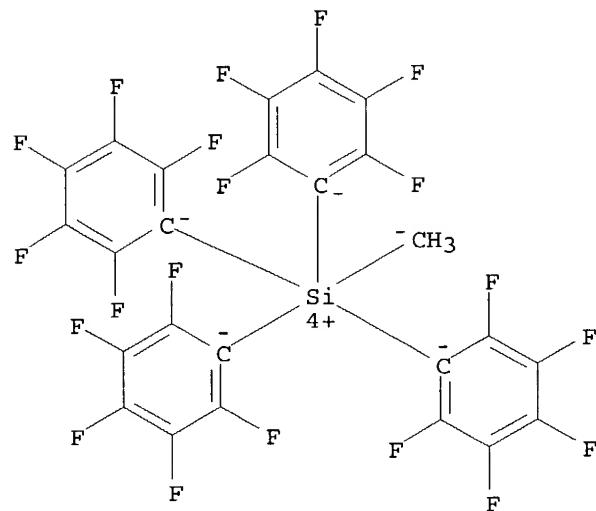
OTHER SOURCE(S): MARPAT 129:149360  
 AB Olefins are polymerized by contact with a transition metal catalyst, wherein the cocatalyst is either XR4 (X = Si, Ge, Sn, Pb; R = H, alkyl, aryl, arylalkyl, alkylaryl; at least one R is not H and contains one or more halogen atoms) or is [X'R'5]-Y+ (X' = Si, Ge, Sn, Pb; R' = H, alkyl, aryl, arylalkyl, alkylaryl; at least one R is not hydrogen and contains one or more halogen atoms; Y+ = cation); the cocatalyst replaces aluminoxanes which can be difficult to remove from polyolefin products. Thus, [(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>SiMe] - [Li(THF)<sub>4</sub>]<sup>+</sup> was prepared and used with bis(cyclopentadienyl)zirconium monohydride monochloride and trioctylaluminum to polymerize ethylene.  
 IT 1524-78-3P, Tetrakis(pentafluorophenyl)silane  
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
 (cocatalyst intermediate; organosilane cocatalysts for polymerization of ethylene)  
 RN 1524-78-3 CAPLUS  
 CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 210771-45-2DP, reaction products with triphenylchloromethane  
210771-45-2P  
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);  
USES (Uses)  
(cocatalyst; organosilane cocatalysts for polymerization of ethylene)  
RN 210771-45-2 CAPLUS  
CN Lithium(1+), tetrakis(tetrahydrofuran)-, (T-4)-,  
methyltetrakis(pentafluorophenyl) silicate(1-) (9CI) (CA INDEX NAME)

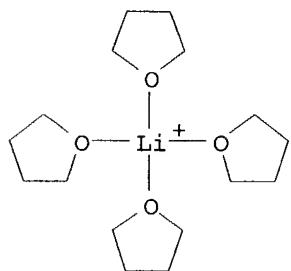
CM 1

CRN 210771-44-1  
CMF C25 H3 F20 Si  
CCI CCS



CM 2

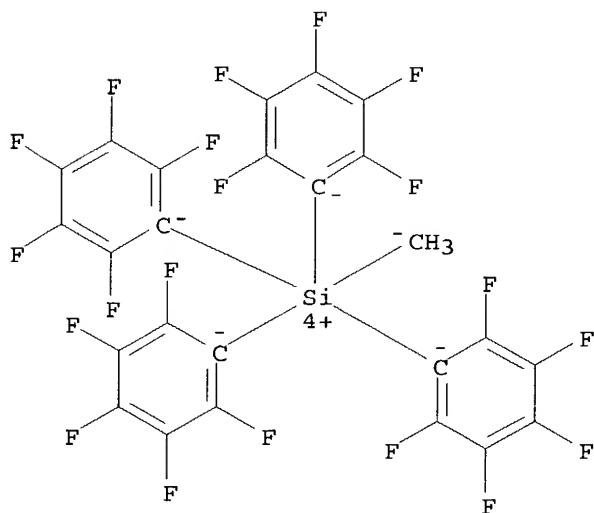
CRN 48186-27-2  
CMF C16 H32 Li O4  
CCI CCS



RN 210771-45-2 CAPLUS  
CN Lithium(1+), tetrakis(tetrahydrofuran)-, (T-4)-,  
methyltetrakis(pentafluorophenyl)silicate(1-) (9CI) (CA INDEX NAME)

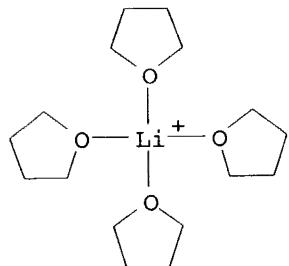
CM 1

CRN 210771-44-1  
CMF C25 H3 F20 Si  
CCI CCS



CM 2

CRN 48186-27-2  
CMF C16 H32 Li O4  
CCI CCS



IC ICM C08F004-60  
ICS C08F010-00; C07F007-08  
CC 35-3 (Chemistry of Synthetic High Polymers)  
ST ethylene polymer catalyst organosilane organozirconium; polyolefin prodn  
catalyst silicon germanium  
IT Polymerization catalysts  
(metallocene; organosilane and -germane cocatalysts for polymerization of  
olefins)  
IT Polymerization catalysts  
(organosilane and -germane catalysts for polymerization of olefins)  
IT Polyolefins  
RL: IMF (Industrial manufacture); PREP (Preparation)  
(organosilane and -germane cocatalysts for polymerization of olefins)  
IT 67108-80-9, Bis(pentamethylcyclopentadienyl)dimethylzirconium  
RL: CAT (Catalyst use); USES (Uses)  
(catalyst; organogermanium cocatalysts for polymerization of ethylene)  
IT 1070-00-4, Trioctylaluminum 37342-97-5 178762-91-9 210771-60-1  
RL: CAT (Catalyst use); USES (Uses)  
(catalyst; organosilane cocatalysts for polymerization of ethylene)  
IT 5121-90-4P  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(cocatalyst intermediate; organosilane and -germane cocatalysts for  
polymerization of ethylene)  
IT 1524-78-3P, Tetrakis(pentafluorophenyl)silane  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(cocatalyst intermediate; organosilane cocatalysts for polymerization of  
ethylene)  
IT 10038-98-9P, Tetrachlorogermane  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(cocatalyst starting material; organogermanium cocatalysts for  
polymerization  
of ethylene)

IT 917-54-4, Methylolithium 1074-91-5, 1-Bromo-2,3,4,5-tetrafluorobenzene  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cocatalyst starting material; organosilane and -germane cocatalysts  
for polymerization of ethylene)

IT 344-04-7, Pentafluorobromobenzene 10026-04-7, Tetrachlorosilane  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cocatalyst starting material; organosilane cocatalysts for polymerization  
of  
ethylene)

IT 13628-95-0P  
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);  
USES (Uses)  
(cocatalyst; organogermanium cocatalysts for polymerization of ethylene)

IT 1452-12-6P, Tetrakis(pentafluorophenyl)germane  
RL: CAT (Catalyst use); IMF (Industrial manufacture); RCT (Reactant); PREP  
(Preparation); RACT (Reactant or reagent); USES (Uses)  
(cocatalyst; organogermanium cocatalysts for polymerization of ethylene)

IT 210771-66-7DP, reaction products with triphenylchloromethane  
210771-66-7P  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(cocatalyst; organogermanium cocatalysts for polymerization of ethylene)

IT 210771-45-2DP, reaction products with triphenylchloromethane  
210771-45-2P 210771-81-6P  
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);  
USES (Uses)  
(cocatalyst; organosilane cocatalysts for polymerization of ethylene)

IT 52910-17-5P  
RL: CAT (Catalyst use); IMF (Industrial manufacture); RCT (Reactant); PREP  
(Preparation); RACT (Reactant or reagent); USES (Uses)  
(cocatalyst; organosilane cocatalysts for polymerization of ethylene)

IT 76-83-5DP, Triphenylchloromethane, reaction products with organosilanes  
and organogermanes  
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);  
USES (Uses)  
(cocatalysts; organosilane and -germane cocatalysts for polymerization of  
ethylene)

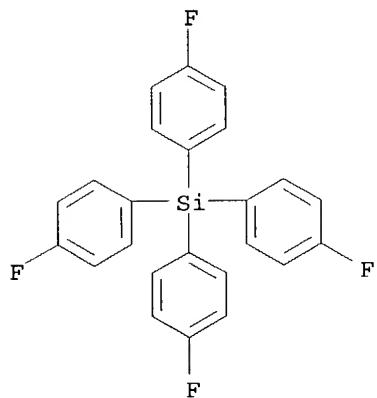
IT 210771-81-6DP, reaction products with triphenylchloromethane  
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);  
USES (Uses)  
(cocatalysts; organosilane cocatalysts for polymerization of ethylene)

IT 925-90-6, Ethylmagnesium bromide  
RL: NUU (Other use, unclassified); USES (Uses)  
(in preparation of organosilane cocatalysts for polymerization of ethylene)

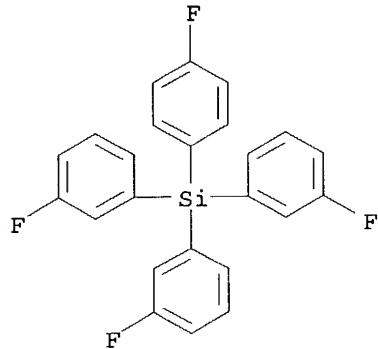
IT 9002-88-4P  
RL: IMF (Industrial manufacture); PREP (Preparation)  
(organosilane and -germane cocatalysts for polymerization of ethylene)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

DOCUMENT NUMBER: 124:261208  
TITLE: Substituent effect on electronegativity of Ar<sub>3</sub>Si and Ar<sub>3</sub>Sn groups: comparison of the results of ab initio quantum-chemical calculations with <sup>19</sup>F NMR data for Ar<sub>3</sub>MQC<sub>6</sub>H<sub>4</sub>F-4 compounds  
AUTHOR(S): Kravtsov, D. N.; Peregudov, A. S.; Shcherbakova, O. V.; Borisov, Yu. A.  
CORPORATE SOURCE: A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, 117813, Russia  
SOURCE: Izvestiya Akademii Nauk, Seriya Khimicheskaya (1995), (10), 1921-4  
CODEN: IASKEA  
PUBLISHER: Institut Organicheskoi Khimii im. N. D. Zelinskogo Rossiiskoi Akademii Nauk  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
AB Ab initio calcns. for the group electronegativity  $\chi$  of Ar<sub>3</sub>Si and Ar<sub>3</sub>Sn groups containing 13 types of m-, p- and polysubstituted Ph groups was performed. The calculated values of  $\chi$ (Ar<sub>3</sub>Si) and  $\chi$ (Ar<sub>3</sub>Sn) correlate better with the  $\sigma_0$  Taft consts. than with  $\sigma$  Hammett consts., which provides evidence for the inductive effect of aryl groups. Good correlation was found for <sup>19</sup>F chemical shifts in Ar<sub>3</sub>SiC<sub>6</sub>H<sub>4</sub>F-4, Ar<sub>3</sub>SnC<sub>6</sub>H<sub>4</sub>F-4, Ar<sub>3</sub>SnCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>F-4 and Ar<sub>3</sub>SnSC<sub>6</sub>H<sub>4</sub>F-4 with the corresponding values of  $\chi$ (Ar<sub>3</sub>Si) and  $\chi$ (Ar<sub>3</sub>Sn).  
IT 63523-07-9 175029-06-8  
RL: PRP (Properties)  
(substituent effect on electronegativity of triarylsilyl and triarylstannyl groups in substituted fluorobenzenes)  
RN 63523-07-9 CAPLUS  
CN Silane, tetrakis(4-fluorophenyl)- (9CI) (CA INDEX NAME)



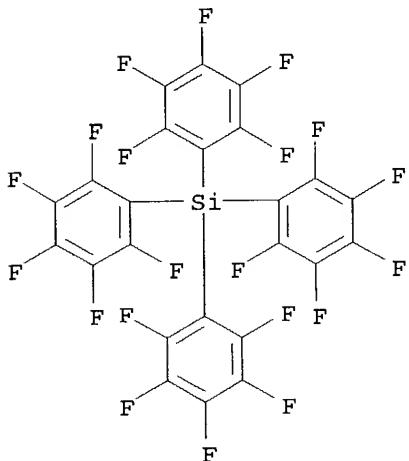
RN 175029-06-8 CAPLUS  
CN Silane, tris(3-fluorophenyl)(4-fluorophenyl)- (9CI) (CA INDEX NAME)



CC 29-8 (Organometallic and Organometalloidal Compounds)  
Section cross-reference(s): 22  
ST group electronegativity silyl stannyl substituent effect; triarylsilyl group electronegativity substituent effect; triarylstannyl group electronegativity substituent effect; Taft substituent const triarylstannyl triarylsilyl group  
IT Electronegativity  
Linear free energy relationship  
Substituent effect  
(substituent effect on electronegativity of triarylsilyl and triarylstannyl groups)  
IT Molecular orbital  
(MNDO, of triarylstannyl- and triarylsilyl-substituted fluorobenzenes)  
IT Substituent constant  
(Taft, substituent effect on electronegativity of triarylsilyl and triarylstannyl groups)  
IT Functional groups  
(silyl, triarylsilyl; substituent effect on electronegativity of triarylsilyl and triarylstannyl groups)  
IT Functional groups  
(stannyl, triarylstannyl; substituent effect on electronegativity of triarylsilyl and triarylstannyl groups)  
IT 426-81-3 1251-03-2 34243-46-4 38186-04-8 51053-80-6 51053-81-7  
51053-82-8 51053-83-9 51107-58-5 51107-59-6 51107-60-9  
51107-61-0 51107-62-1 51107-63-2 63523-02-4 63523-03-5  
63523-04-6 63523-05-7 63523-06-8 63523-07-9 63523-08-0  
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78795-74-1 84761-46-6 84761-47-7 84761-48-8 84761-49-9  
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175029-06-8 175029-07-9  
RL: PRP (Properties)  
(substituent effect on electronegativity of triarylsilyl and triarylstannyl groups in substituted fluorobenzenes)

L59 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1996:58862 CAPLUS

DOCUMENT NUMBER: 124:232542  
TITLE: A convenient preparation of pentafluorophenyl(fluoro)silanes: reactivity of pentafluorophenyltrifluorosilane  
AUTHOR(S): Frohn, H. J.; Giesen, M.; Klose, A.; Lewin, A.; Bardin, V. V.  
CORPORATE SOURCE: Fachgebiet Anorganische Chemie, Gerhard-Mercator-Universitaet Duisburg, Lotharstr. 1, Duisburg, D-47048, Germany  
SOURCE: Journal of Organometallic Chemistry (1996), 506(1-2), 155-64  
CODEN: JORCAI; ISSN: 0022-328X  
PUBLISHER: Elsevier  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 124:232542  
AB Pentafluorophenyl(fluoro)silanes ( $C_6F_5$ ) $_n$ SiF $_4-n$  ( $n = 1, 2$ ) were prepared from the corresponding ethoxysilanes by sequential chlorodeethoxylation with SOCl $_2$  and fluoridation of chlorosilanes with SbF $_3$ . The conversion of C $_6$ F $_5$ Si(OEt) $_3$  and C $_6$ F $_5$ SiCl $_3$  into C $_6$ F $_5$ SiF $_3$  with anhydrous HF is described. Some reactions of C $_6$ F $_5$ SiF $_3$  with electrophiles and nucleophiles were studied.  
IT 1524-78-3, Tetrakis(pentafluorophenyl) silane  
RL: PRP (Properties)  
(NMR)  
RN 1524-78-3 CAPLUS  
CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)  
ST pentafluorophenylfluorosilane prep reaction; silane  
pentafluorophenylfluoro prep reaction; ethoxysilane chlorodeethoxylation  
fluoridation  
IT Fluorination  
(of pentafluorophenyl(chloro)silanes)

IT Silanes  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(pentafluorophenyl(fluoro)silanes; preparation and reactions with electrophiles and nucleophiles)

IT Ethoxylation  
(retro, chloro-; of pentafluorophenyl(ethoxy)silanes)

IT 1524-78-3, Tetrakis(pentafluorophenyl)silane 20160-39-8,  
Chlorotris(pentafluorophenyl)silane 35370-01-5,  
Fluorotris(pentafluorophenyl)silane  
RL: PRP (Properties)  
(NMR)

IT 371-20-0P, Diethoxy(fluoro)borane 86802-17-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(formation from pentafluorophenyltriethoxysilane and boron fluoride etherate)

IT 344-04-7P, Bromopentafluorobenzene 174743-13-6P,  
Bromodifluoro(pentafluorophenyl)silane  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(formation from pentafluorophenyltrifluorosilane and bromine)

IT 14188-35-3P, Dibromodifluorosilane 18356-67-7P, Tribromo(fluoro)silane  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(formation from pentafluorophenyltrifluorosilane and bromine/aluminum bromide)

IT 7783-61-1P, Silicon tetrafluoride 121827-61-0P,  
Bis(pentafluorophenyl)iodonium  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(formation from pentafluorophenyltrifluorosilane and fluoroiodonium fluoroantimonate)

IT 20160-47-8P, Chloro(ethoxy)bis(pentafluorophenyl)silane 174743-04-5P,  
Ethoxydifluoro(pentafluorophenyl)silane 174743-05-6P,  
Diethoxy(fluoro)(pentafluorophenyl)silane 174743-08-9P,  
Dichloro(ethoxy)(pentafluorophenyl)silane  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; convenient preparation of fluorophenyl(fluoro)silanes: reactivity of fluorophenylfluorosilane)

IT 174743-11-4P, Dibutyl(ethoxy)(pentafluorophenyl)silane  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with acetyl chloride/zinc chloride)

IT 20083-38-9P, Trichloro(pentafluorophenyl)silane 20160-45-6P,  
Dichlorobis(pentafluorophenyl)silane  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction with antimony fluoride)

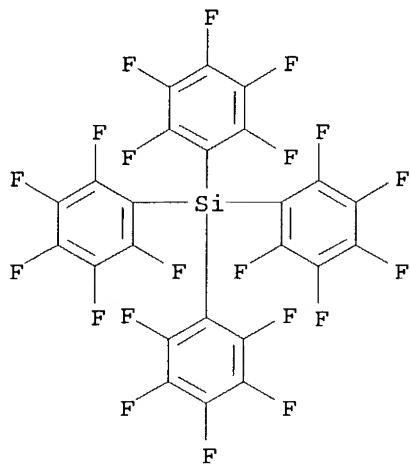
IT 5272-26-4P, Trifluoro(pentafluorophenyl)silane  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reactions with electrophiles and nucleophiles)

IT 27585-17-7P, Difluorobis(pentafluorophenyl)silane  
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and reactions with electrophiles and nucleophiles)  
IT 174743-06-7P, Difluoro(pentafluorophenyl)(1-piperidino)silane  
174743-07-8P, Fluoro(pentafluorophenyl)bis(1-piperidino)silane  
174743-09-0P, Tributyl(pentafluorophenyl)silane 174743-10-3P,  
Dibutyl(fluoro)(pentafluorophenyl)silane 174743-12-5P,  
Dibutyl(4-butyltetrafluorophenyl)(pentafluorophenyl)silane  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
IT 693-03-8, Bromo(butyl)magnesium  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with pentafluorophenyltrifluorosilane)  
IT 13888-69-2, Diethoxybis(pentafluorophenyl)silane  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with thionyl chloride/pyridinium chloride)  
IT 20083-34-5, Triethoxy(pentafluorophenyl)silane  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactions with hydrofluoric acid, thionyl chloride/pyridinium  
chloride, boron fluoride and other reagents)  
IT 109-72-8, Butyllithium, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactions with pentafluorophenyltrifluorosilane)

L59 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:602108 CAPLUS  
DOCUMENT NUMBER: 117:202108  
TITLE: Thermodynamic simulation of deposition of molybdenum  
and tungsten disilicides in metalorganic CVD processes  
AUTHOR(S): Kuznetsov, F. A.; Titov, V. A.; Golubenko, A. N.;  
Titov, A. A.  
CORPORATE SOURCE: Inst. Inorg. Chem., Novosibirsk, 630090, USSR  
SOURCE: Proceedings of SPIE-The International Society for  
Optical Engineering (1992), 1783(Int. Conf.  
Microelectron., 1992), 541-50  
CODEN: PSISDG; ISSN: 0277-786X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Modeling of disilicide deposition in the systems with volatile metalorg.  
and fluorinated Si organic compds. was performed for a number of systems  
M-Si-C-H-Ar, M-Si-C-O-Cl-H-Ar, M-Si-C-H-F-Ar, M-Si-C-O-F-H-Ar (M = W, Mo).  
In some of these systems (especially with fluorinated compds.) there are wider  
regions of quasi-equilibrium deposition of disilicides.  
IT 1524-78-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with tungsten cyclopentadienyl complex in tungsten  
disilicide deposition)  
RN 1524-78-3 CAPLUS  
CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 75-1 (Crystallography and Liquid Crystals)  
Section cross-reference(s): 69  
ST deposition molybdenum tungsten silicide metalorg simulation  
IT Vapor deposition processes  
    (of molybdenum and tungsten disilicide, thermodn. simulation of  
    metalorg.)  
IT 12039-88-2, Tungsten silicide (WSi<sub>2</sub>) 12136-78-6, Molybdenum silicide  
(MoSi<sub>2</sub>)  
    RL: PEP (Physical, engineering or chemical process); PROC (Process)  
        (deposition of, thermodn. simulation of metalorg. vapor-phase)  
IT 1271-33-6  
    RL: RCT (Reactant); RACT (Reactant or reagent)  
        (reaction of, with silicon compds. in tungsten disilicide deposition)  
IT 1524-78-3 122571-42-0  
    RL: RCT (Reactant); RACT (Reactant or reagent)  
        (reaction of, with tungsten cyclopentadienyl complex in tungsten  
        disilicide deposition)  
  
L59 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1992:539948 CAPLUS  
DOCUMENT NUMBER: 117:139948  
TITLE: Photoelectron helium spectra of the pentafluorophenyl  
derivatives of Group IV and V elements  
AUTHOR(S): Petrachenko, N. E.; Vovna, V. I.; Furin, G. G.  
CORPORATE SOURCE: Nauchno-Issled. Fiz.-Tekh.-Inst., Vladivostok, Russia  
SOURCE: Zhurnal Fizicheskoi Khimii (1992), 66(2), 515-20  
CODEN: ZFKHA9; ISSN: 0044-4537  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
AB In the compds. of tricoordinated P and As, intramol. interaction is observed  
of a lone electron pair with the  $\pi$ -MO fluorinated benzene ring, while  
in the P-containing compds. this interaction is stronger, than in As-containing  
compds. In tetracoordinated compds., the interaction between orbitals of  
the group X = O (X=P,As) with groups of  $\pi$ -MO substituents was not observed

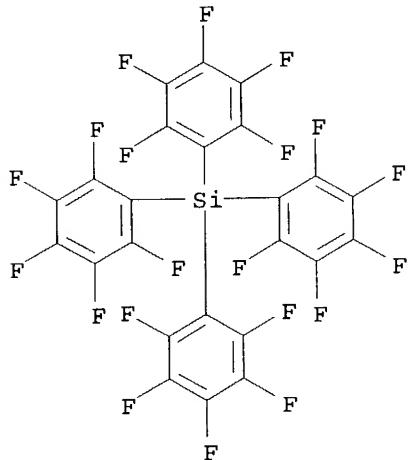
The basic contribution to the bonding is from  $\sigma$ -orbitals localized on X-C bonds.

IT 1524-78-3

RL: PRP (Properties)  
(photoelectron spectrum of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 73-6 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

ST photoelectron fluorophenyl Group IVA VA deriv; phenyl fluoro Group IVA VA photoelectron; bonding fluorophenyl Group IVA VA deriv

IT Bond  
(in fluorophenyl derivs. of Group IVA and VA elements)

IT Photoelectron spectroscopy  
(of pentafluorophenyl derivs. of Group IVA and VA elements)

IT 1065-49-2 1259-34-3 1259-35-4, Tris(pentafluorophenyl)phosphine  
1452-12-6 1524-78-3 2729-11-5, Tris(pentafluorophenyl)phosphine oxide  
18005-77-1

RL: PRP (Properties)  
(photoelectron spectrum of)

L59 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:534254 CAPLUS

DOCUMENT NUMBER: 111:134254

TITLE: Reactions of arylmethylsilanes and tetraarylsilanes with xenon difluoride in the presence of fluoride ions

AUTHOR(S): Bardin, V. V.; Stennikova, I. V.; Furin, G. G.;  
Leshina, T. V.; Yakobson, G. G.

CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR

SOURCE: Zhurnal Obshchey Khimii (1988), 58(11), 2580-8  
CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S) : CASREACT 111:134254

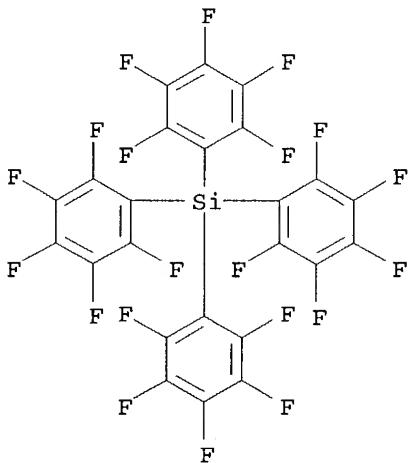
AB The reaction of RnSiMe4-n (R = C6F5, p-F3CC6F4, tetrafluoro-4-pyridyl; n = 1, 2, 4) with XeF2 in the presence of MF (M = K, Rb, Cs) gave protodesilylation products and diaryls. The reaction is a convenient method for generation of polyfluoroaryl and polyfluorohetaryl radicals under mild conditions.

IT 1524-78-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with xenon difluoride)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s) : 25, 27

ST arylmethylsilane xenon difluoride reaction; pyridylmethylsilane xenon difluoride reaction; xenon difluoride fluoroaryl methylsilane reaction; protodesilylation arylmethylsilane xenon difluoride reaction; radical polyfluoroaryl polyfluorohetaryl

IT Heterocyclic compounds

RL: PROC (Process)  
(aromatic, fluoro, radicals, generation of, from reaction of hetaryl methylsilanes with xenon difluoride)

IT Aromatic hydrocarbons, preparation

RL: PREP (Preparation)  
(fluoro, radicals, generation of, from reaction of arylmethylsilanes with xenon difluoride)

IT Silylation

(retro, in reaction of arylmethylsilanes with xenon difluoride)

IT 768-32-1, Trimethylphenylsilane 1048-08-4, Tetraphenylsilane  
3728-43-6, Trimethyl-p-tolylsilane 4405-33-8, Trimethyl-p-nitrophenylsilane

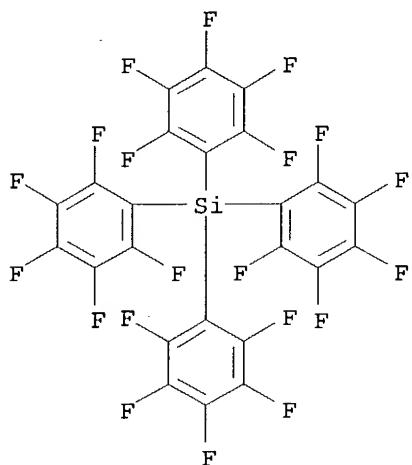
RL: RCT (Reactant); RACT (Reactant or reagent)

(attempted reaction of, with xenon difluoride)

IT 92-52-4P, 1,1'-Biphenyl, preparation 98-08-8P 344-04-7P 363-72-4P

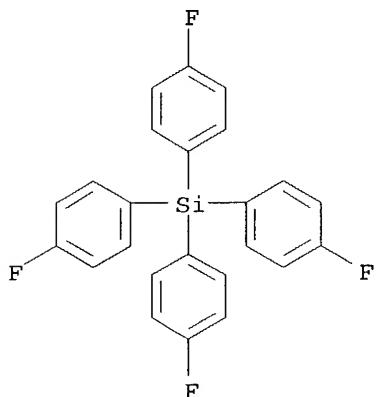
434-90-2P 581-80-6P 651-80-9P 2875-18-5P 2875-19-6P 3511-91-9P  
17823-47-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
IT 7789-23-3, Potassium fluoride 13400-13-0, Cesium fluoride 13446-74-7,  
Rubidium fluoride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of arylmethyldisilanes with xenon difluoride in presence of)  
IT 13709-36-9, Xenon difluoride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with arylmethyldisilanes)  
IT 75-25-2, Tribromomethane  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with trimethylpentaphenylsilane and xenon  
difluoride)  
IT 312-75-4 1206-46-8 1524-78-3 16297-29-3 122571-41-9  
122571-42-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with xenon difluoride)

L59 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1984:510434 CAPLUS  
DOCUMENT NUMBER: 101:110434  
TITLE: Pentafluorophenyliodine(V) compounds, part 1.  
Preparation of pentafluorophenyliodine tetrafluoride  
and other aryliodine tetrafluorides by reaction of  
iodine pentafluoride with arylsilanes  
AUTHOR(S): Frohn, Hermann Josef  
CORPORATE SOURCE: Fachber.-Chem., Univ. Gesamthochsch. Duisburg,  
Duisburg, 4100/1, Fed. Rep. Ger.  
SOURCE: Chemiker-Zeitung (1984), 108(4), 146-7  
CODEN: CMKZAT; ISSN: 0009-2894  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
OTHER SOURCE(S): CASREACT 101:110434  
AB RIF<sub>4</sub> (R = C<sub>6</sub>F<sub>5</sub>, Ph, p-F, -Me-, -MeOC<sub>6</sub>H<sub>4</sub>) were prepared by treating IF<sub>5</sub> with  
RnSiX<sub>4-n</sub> (X = F, Me; n = 1-4). The effect of solvent and pyridine on the  
reaction was studied.  
IT 1524-78-3 63523-07-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with iodine pentafluoride)  
RN 1524-78-3 CAPLUS  
CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 63523-07-9 CAPLUS

CN Silane, tetrakis(4-fluorophenyl)- (9CI) (CA INDEX NAME)



CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 29

ST fluorophenyliodine tetrafluoride; phenyliodine tetrafluoride; iodine pentafluorophenyl tetrafluoride; silane phenyl iodine pentafluoride reaction

IT Solvent effect

(on reaction of iodine pentafluoride with phenylsilanes)

IT 22121-26-2P 22121-27-3P 29848-54-2P 38091-68-8P 91679-75-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 110-86-1, uses and miscellaneous

RL: USES (Uses)

(reaction of iodine pentafluoride with phenylsilanes in presence of)

IT 368-47-8 1048-08-4 1206-46-8 1524-78-3 5272-26-4

10256-83-4 10536-62-6 13688-78-3 24727-90-0 35370-01-5

50625-30-4 63523-07-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with iodine pentafluoride)

IT 7783-66-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phenylsilanes)

IT 75-05-8, uses and miscellaneous  
RL: PRP (Properties)  
(solvent effect of, on reaction of iodine pentafluoride with  
phenylsilanes)

L59 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1978:624407 CAPLUS

DOCUMENT NUMBER: 89:224407

TITLE: The crystal structure of tetrakis(pentafluorophenyl) silane

AUTHOR(S): Karipides, Anastas; Foerst, Barbara

CORPORATE SOURCE: Dep. Chem., Miami Univ., Oxford, OH, USA

SOURCE: Acta Crystallographica, Section B: Structural

Crystallography and Crystal Chemistry (1978), B34(11),  
3494-6

CODEN: ACBCAR; ISSN: 0567-7408

DOCUMENT TYPE: Journal

LANGUAGE: English

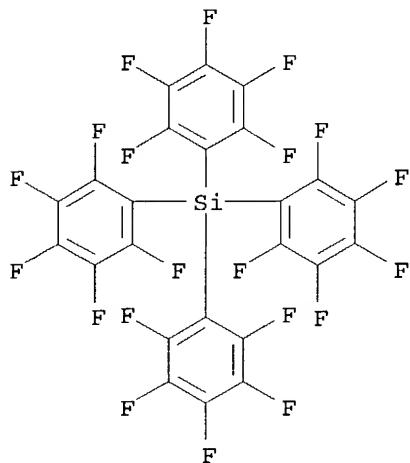
AB The crystal structure of (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Si was determined from 3-dimensional single-crystal x-ray data collected on a computer-automated diffractometer. The compound crystallizes in space group I41/a with cell dimensions of a 17.165 (12) and c 8.128 (8) Å; Z = 4. The (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Si mols. have S4 crystallog. imposed symmetry. Full-matrix least squares refinement yielded a conventional R factor of 0.070.

IT 1524-78-3

RL: PRP (Properties)  
(crystal structure of)

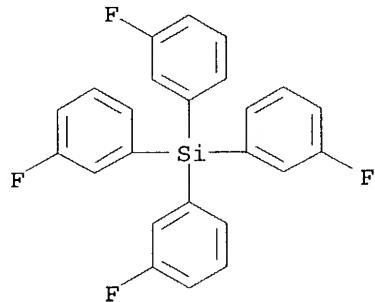
RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

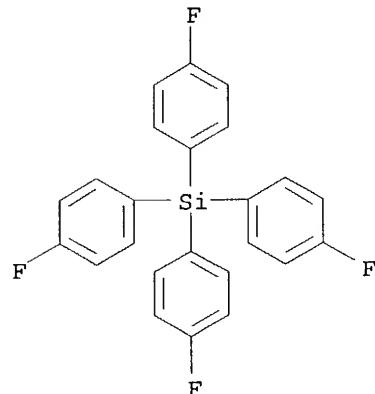


CC 75-5 (Crystallization and Crystal Structure)  
ST structure pentafluorophenylsilane; fluorophenylsilane structure; silane  
pentafluorophenyl structure; phenyl pentafluorosilane structure  
IT Crystal structure  
Molecular structure  
(of tetrakis(pentafluorophenyl)silane)  
IT 1524-78-3  
RL: PRP (Properties)  
(crystal structure of)

L59 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1977:452639 CAPLUS  
DOCUMENT NUMBER: 87:52639  
TITLE: A fluorine-19 NMR investigation of the transmission of  
electronic effects in triaryl(4-fluorophenyl)silanes  
AUTHOR(S): Pombrik, S. I.; Kravtsov, D. N.; Peregudov, A. S.;  
Fedin, E. I.; Nesmeyanov, A. N.  
CORPORATE SOURCE: Inst. Organo-Elem. Compd., Moscow, USSR  
SOURCE: Journal of Organometallic Chemistry (1977), 131(3),  
355-63  
CODEN: JORCAI; ISSN: 0022-328X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB For the title compds., a linear relation between the F chemical shifts and  
the  $\Sigma\sigma_0$  values of the substituted phenyl groups attached to  
the S atom has been found. The transmission of electronic effects from  
one aromatic ring to another in tetraarylsilanes occurs mainly by an  
inductive mechanism. The transmitting ability of Si-C bonds is somewhat  
higher than that of Sn-C bonds.  
IT 3869-53-2 63523-07-9  
RL: PRP (Properties)  
(fluorine-19 NMR spectrum of)  
RN 3869-53-2 CAPLUS  
CN Silane, tetrakis(3-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 63523-07-9 CAPLUS  
CN Silane, tetrakis(4-fluorophenyl)- (9CI) (CA INDEX NAME)



CC 22-9 (Physical Organic Chemistry)  
ST fluorine NMR silane; LFER NMR fluorophenylsilane  
IT Linear free energy relationship  
(in fluorine-19 NMR spectra of triaryl(4-fluorophenyl)silanes)  
IT Nuclear magnetic resonance  
(of fluorine-19, in triaryl(fluorophenyl)silanes, substituent effect  
in)  
IT 3869-53-2 63523-02-4 63523-03-5 63523-04-6 63523-05-7  
63523-06-8 63523-07-9 63523-08-0 63523-09-1 63523-10-4  
63523-11-5  
RL: PRP (Properties)  
(fluorine-19 NMR spectrum of)  
IT 349-91-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and reaction of, with trichlorobromobenzene)  
IT 13190-50-6 21928-51-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with (fluorophenyl)trichlorosilane)

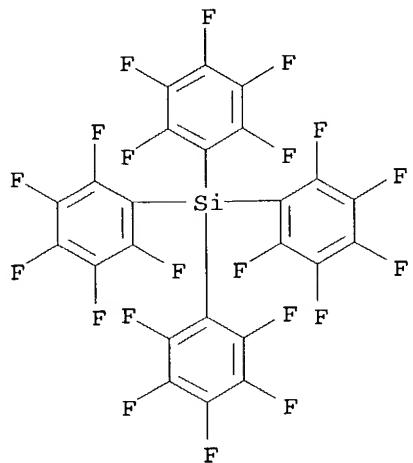
IT 76-86-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with bromofluorobenzene)

IT 10026-04-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with fluorophenylmagnesium bromide)

IT 352-13-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with silicon tetrachloride)

IT 460-00-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with triphenylsilane)

L59 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1973:123476 CAPLUS  
DOCUMENT NUMBER: 78:123476  
TITLE: NMR studies of pentafluorophenyl-substituted silanes.  
I. Relations between chemical shifts, coupling  
constants, and (p-d) $\pi$  interactions  
AUTHOR(S): Haegele, Gerhard; Weidenbruch, Manfred  
CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Duesseldorf, Duesseldorf,  
Fed. Rep. Ger.  
SOURCE: Chemische Berichte (1973), 106(2), 460-70  
CODEN: CHBEAM; ISSN: 0009-2940  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
AB The 60-100 MHz  $^{19}\text{F}$ -NMR spectra of 21 silanes  $\text{RnSiX}_4\text{-n}$  ( $\text{R} = \text{C}_6\text{F}_5$ ,  $n = 1-4$ ,  
 $\text{X} = \text{H}$ , alkyl, halo, or amino),  $\text{RSiMe}_2\text{SiMe}_2\text{R}$ , and  $\text{RSiMe}_2\text{SiMe}_3$  were determined  
and analyzed using [AX]2M approxns. The relations between the title  
parameters were discussed in terms of the  $\pi$ -acceptor action of the SiX  
groups and long-range interannular F-F and F-H couplings.  
IT 1524-78-3  
RL: PRP (Properties)  
(NMR of, fluorine-19 of,  $\pi$  interactions in relation to)  
RN 1524-78-3 CAPLUS  
CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 22-2 (Physical Organic Chemistry)  
ST fluorophenylsilane NMR; silane pentafluorophenyl NMR; fluorine 19 NMR  
fluorophenylsilane; pi acceptor fluorophenylsilane  
IT Conjugation  
(in pentafluorosilanes, NMR in relation to)  
IT Spin, nuclear coupling  
(of fluorine with fluorine, in pentafluorophenylsilanes, conjugation in  
relation to)  
IT Nuclear magnetic resonance  
(of fluorine-19, of pentafluorophenylsilanes, conjugation in relation  
to)  
IT 1206-46-8 1524-78-3 5272-26-4 10536-62-6 17067-70-8  
17067-71-9 18920-98-4 20160-39-8 21655-08-3 27585-17-7  
35369-97-2 35369-98-3 35370-01-5  
RL: PRP (Properties)  
(NMR of, fluorine-19 of, π interactions in relation to)  
IT 7782-41-4, properties  
RL: PRP (Properties)  
(NMR of, in pentafluorophenylsilanes)  
IT 13888-77-2 20160-40-1 23761-73-1 23761-74-2 23761-75-3  
23761-76-4 27490-05-7 27491-93-6 33558-55-3 33558-56-4  
RL: PRP (Properties)  
(NMR of, π interactions in relation to fluorine in)

L59 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1969:119359 CAPLUS  
DOCUMENT NUMBER: 70:119359  
TITLE: Fragmentation and rearrangement processes in the mass  
spectra of perhalogenoaromatic compounds. II.  
Pentafluorophenyl derivatives of group IV  
AUTHOR(S): Miller, Jack M.  
CORPORATE SOURCE: Brock Univ., St. Catharines, ON, Can.  
SOURCE: Canadian Journal of Chemistry (1969), 47(10), 1613-20  
CODEN: CJCHAG; ISSN: 0008-4042

DOCUMENT TYPE: Journal  
LANGUAGE: English

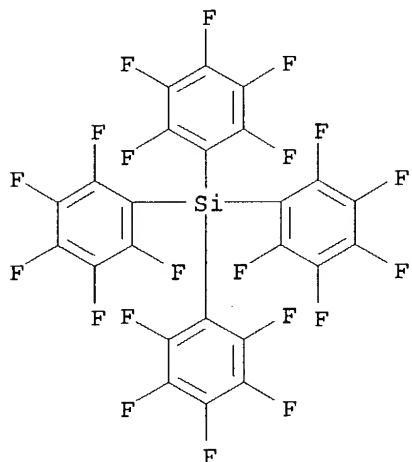
AB The mass spectra of compds. of the type  $(C_6F_5)_4M$  ( $M = Si, Ge, Sn, and Pb$ ) have been studied. Bond forming rearrangements were detected, involving F abstraction by the central atom, forming perfluorophenylene ions and neutral metal fluoride species. The heavier metals give simpler spectra and fragmentation schemes. The bulk of the ion current is carried by fluorocarbon ions for the Si derivative and by organometallic or metal fluoride ions in the other three cases,  $SnF^+$  and  $PbF^+$  forming the base peaks in their spectra. When M is C in the compds.  $(C_6F_5)_3COH$  and  $(C_6F_5)_2CO$  there is little evidence for rearrangements and transfer of F to the central C atom.

IT 1524-78-3

RL: PRP (Properties)  
(mass spectrum of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 71 (Electric Phenomena)

ST perhaloaroms mass spectra; silicon perfluorophenyls mass spectra; germanium perfluorophenyls mass spectra; tin perfluorophenyls mass spectra; lead perfluorophenyls mass spectra; perfluorophenyls mass spectra; fluorophenyls mass spectra

IT Mass spectra

(of Group IVA fluorophenyl derivs.)

IT 1065-49-2 1111-02-0 1452-12-6 1524-78-3

RL: PRP (Properties)  
(mass spectrum of)

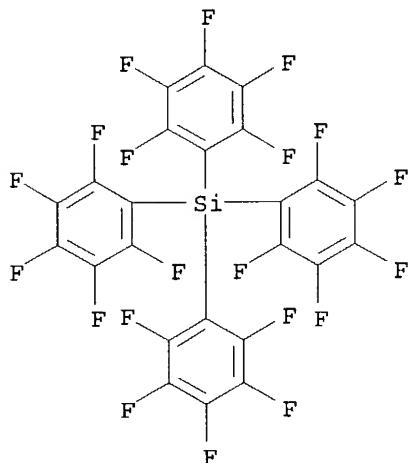
L59 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1968:477334 CAPLUS

DOCUMENT NUMBER: 69:77334

TITLE: A direct preparation of some pentafluorophenyl-containing silanes

AUTHOR(S): Whittingham, A.; Jarvie, A. W. P.  
CORPORATE SOURCE: Univ. Aston, Birmingham, UK  
SOURCE: Journal of Organometallic Chemistry (1968), 13(1),  
125-9  
CODEN: JORCAI; ISSN: 0022-328X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The reaction of pentafluorobromobenzene with both tetraethoxysilane and tetrachlorosilane, by a modified Grignard method, leads to the formation of compds. of the type  $(C_6F_5)_nSiX_4-n$  (X = OEt and Cl and n = 1 - 4). These compds. have been characterized by phys. methods, elemental anal., interconversion and the preparation of derivs.  
IT 1524-78-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 1524-78-3 CAPLUS  
CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)  
ST silanes perfluorophenyl; silicon org compds  
IT 1206-46-8P 1524-78-3P 10536-62-6P 13888-69-2P 20083-34-5P  
20083-38-9P 20160-45-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

L59 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1968:456104 CAPLUS  
DOCUMENT NUMBER: 69:56104  
TITLE: The fluorine-19 NMR spectra of some pentafluorophenyl compounds of group IV elements  
AUTHOR(S): Jolley, K. W.; Sutcliffe, L. H.  
CORPORATE SOURCE: Univ. Liverpool, Liverpool, UK  
SOURCE: Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (1968), 24(8), 1191-203

CODEN: SAMCAS; ISSN: 1386-1425

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Accurate chemical shifts were determined for the pentafluorophenyl F nuclei of  
a

number of Group IV pentafluorophenyl compds. by the use of an extended lock  
in the HA mode. All the compds. studied have a very large ortho shift,  
the trends of which can be predicted by both the van der Waals elec. field  
theory and the through bond theory of Hruska, et al. The m- and p-19F  
chemical shifts were used to predict the  $\pi$ -electron accepting ability of  
the various substituents attached to the Group IV atom. The coupling  
consts. obtained from those compds. which give resolvable spectra supports  
the chemical shift work. 35 references.

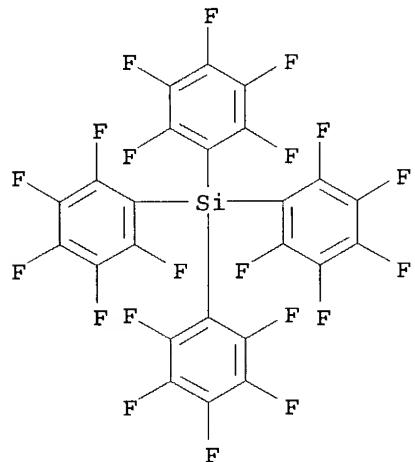
IT 1524-78-3

RL: PRP (Properties)

(nuclear magnetic resonance of fluorine in)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 73 (Spectra and Other Optical Properties)

ST NMR F 19 fluorophenyls; fluorine 19 NMR; fluorophenyls NMR

IT Substituents

(electron accepting ability of, of Group IV compds., N.M.R. in determination  
of)

IT Electron acceptors

(nuclear magnetic resonance in determination of)

IT Nuclear magnetic resonance

(of fluorine, in (pentafluorophenyl) derivs. of Group IV elements)

IT 801-79-6 1015-53-8 1058-08-8 1062-67-5 1062-71-1 1065-49-2  
1080-51-9 1106-04-3 1111-02-0 1259-89-8 1262-57-3 1452-12-6  
1524-78-3 10177-67-0 10177-68-1 10177-69-2 10360-39-1

RL: PRP (Properties)

(nuclear magnetic resonance of fluorine in)

L59 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1968:13065 CAPLUS  
 DOCUMENT NUMBER: 68:13065  
 TITLE: Polyhalo-organometallic and -organometalloidal compounds. VIII. Preparation of some pentafluorophenyl substituted organosilicon compounds  
 AUTHOR(S): Fearon, F. W. Gordon; Gilman, Henry  
 CORPORATE SOURCE: Iowa State Univ., Ames, IA, USA  
 SOURCE: Journal of Organometallic Chemistry (1967), 10(3), 409-19  
 CODEN: JORCAI; ISSN: 0022-328X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

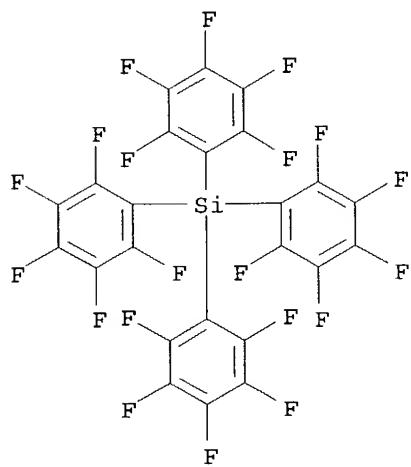
AB The preparation and some properties of  $(C_6F_5)_nSiPh_4-n$  (where n = 1-4) and  $(C_6F_5)_nPh_3-nSiX$  (where n = 1 or 2 and X = H or Cl) are described. In general, these compds. were obtained by the reaction of a (pentafluorophenyl)metallic compound with the corresponding chlorosilane. However,  $(C_6F_5)_nPh_3-nSiCl$  could not be obtained in this manner; they were prepared by the chlorination of the corresponding organosilicon hydrides. Evidence is presented which suggests that  $C_6Cl_5Li$  is more reactive towards  $ClSiPh_3$  than is  $C_6F_5Li$  under similar conditions. The reaction of an alkylolithium compound with  $HPh_2SiC_6F_5$  leads predominantly to cleavage of the  $C_6F_5$  group from Si. The ir spectra of all the above compds. are discussed and the uv spectra of  $(C_6F_5)_nSiPh_4-n$  (where n = 1-4) are reported. 18 references.

IT 1524-78-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



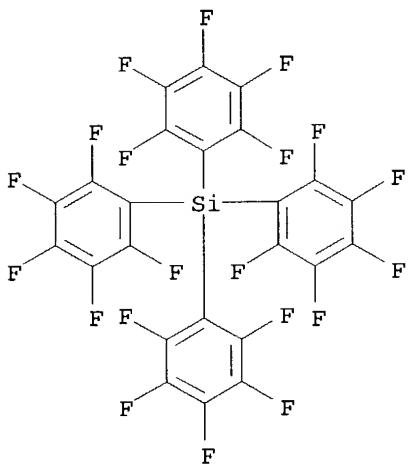
CC 29 (Organometallic and Organometalloidal Compounds)

ST SILANES PENTAFLUOROPHENYL; FLUORO AROM SILANES

IT 1206-46-8P 1524-78-3P 17067-69-5P 17067-70-8P 17067-71-9P

17067-73-1P 17067-74-2P 17067-75-3P 17067-76-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

L59 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1965:498496 CAPLUS  
DOCUMENT NUMBER: 63:98496  
ORIGINAL REFERENCE NO.: 63:18136a-b  
TITLE: Pentafiuorophenyl organometallic compounds of group IV elements  
AUTHOR(S): Tamborski, C.; Soloski, E. J.; Dec, S. M.  
CORPORATE SOURCE: Wright Patterson Air Force Base, Dayton, OH  
SOURCE: Journal of Organometallic Chemistry (1965), 4(6), 446-54  
CODEN: JORCAI; ISSN: 0022-328X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The synthesis of pentafiuorophenyl group IV elements  $(C_6F_5)_4Si$ ,  $(C_6F_5)_4Ge$ ,  $(C_6F_5)_4Sn$ ,  $(C_6F_5)_4Pb$ ,  $(C_5H_5)_2Ti$   $(C_5F_5)_2$  and  $(C_6H_5)_2Zr(C_6F_5)_2$  is reported. The above compounds are prepared through the reaction of the appropriate metal halide and pentafiuorophenyllithium. The various pentafiuorophenyl derivatives are subjected to the following studies: infrared and vapor phase chromatography analysis, acid and base hydrolysis, thermal stability, and reactions with bromine and lithium.  
IT 1524-78-3, Silane, tetrakis(pentafluorophenyl)-  
(preparation of)  
RN 1524-78-3 CAPLUS  
CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 39 (Organometallic and Organometalloidal Compounds)  
IT Organometallic compounds  
(heterocyclic)  
IT Heterocyclic compounds  
(metal complexes)

IT Spectra, infrared  
(of tetrakis(pentafluorophenyl) derivs. of Group IV elements)  
IT 1065-49-2, Tin, tetrakis(pentafluorophenyl)- 1111-02-0, Lead,  
tetrakis(pentafluorophenyl)- 1452-12-6, Germane,  
tetrakis(pentafluorophenyl) 1524-78-3, Silane,  
tetrakis(pentafluorophenyl)- 12097-97-1, Zirconium,  
dicyclopentadienylbis(pentafluorophenyl)- 12155-89-4, Titanium,  
dicyclopentadienylbis(pentafluorophenyl)-  
(preparation of)

L59 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1964:17001 CAPLUS  
DOCUMENT NUMBER: 60:17001  
ORIGINAL REFERENCE NO.: 60:3009f-g  
TITLE: Tetrakis(pentafluorophenyl)silane  
INVENTOR(S): Pummer, Walter J.; Wall, Leo A.  
PATENT ASSIGNEE(S): United States Dept. of the Navy  
SOURCE: 1 p.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
PATENT INFORMATION:

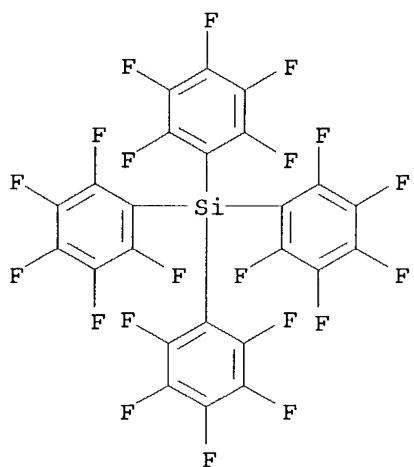
| PATENT NO. | KIND  | DATE     | APPLICATION NO. | DATE     |
|------------|-------|----------|-----------------|----------|
| -----      | ----- | -----    | -----           | -----    |
| US 3109855 |       | 19631105 | US              | 19610626 |

AB Division of U.S. 3,046,313 (CA 57, 15003a). Pentafluorobromobenzene (I) is converted to the Grignard reagent and the Grignard reagent is treated with SiCl<sub>4</sub> to give the title compound, which can be used as a fuel-resistant substance. I (24.7 g.) and a small crystal of iodine are added to a mixture of 2.4 g. Mg in 50 ml. anhydrous ether, the mixture cooled to 0°, 2.83 ml. SiCl<sub>4</sub> added, the mixture agitated 1 hr. at 0°, refluxed 2.5 hrs., and allowed to cool overnight. The mixture is poured into 100 ml. 6N HCl, and the precipitate obtained separated, dried, and sublimed at 208° at 1 mm. to give 5.5 g. tetrakis(pentafluorophenyl)silane, m. 246-8°, 32% yield.

IT 1524-78-3, Silane, tetrakis(pentafluorophenyl)-  
(preparation of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



NCL 260448200  
 CC 39 (Organometallic and Organometalloidal Compounds)  
 IT 1524-78-3, Silane, tetrakis(pentafluorophenyl)-  
 (preparation of)

L59 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:475681 CAPLUS

DOCUMENT NUMBER: 57:75681

ORIGINAL REFERENCE NO.: 57:15003a-f

TITLE: Pentafluoroiodobenzene

INVENTOR(S): Pummer, Walter J.; Wall, Leo A.

PATENT ASSIGNEE(S): U.S. Dept. of the Navy

SOURCE: 3 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

PATENT INFORMATION:

| PATENT NO. | KIND | DATE     | APPLICATION NO. | DATE     |
|------------|------|----------|-----------------|----------|
| US 3046313 |      | 19620724 | US              | 19600503 |

AB Pentafluoroiodobenzene (I), an intermediate in the preparation of perfluorophenyl derivs., was prepared from pentafluorobromobenzene (II) via the Grignard reagent or by iodination of pentafluorobenzene (III). Thus, to a refluxing solution of the Grignard reagent from 10 g. II and 1 g. Mg in 10 ml. Et<sub>2</sub>O was added 9.76 g. F<sub>2</sub>C<sub>1</sub>C<sub>6</sub>H<sub>4</sub>I in 5 ml. Et<sub>2</sub>O, the mixture refluxed 3 hrs., let stand overnight, 50 ml. 6N HCl added, the Et<sub>2</sub>O layer separated, dried, and distilled to give 5.78 g. I, b<sub>35</sub> 77-8°, n<sub>20D</sub> 1.4990. In another example the same amount of Grignard-reagent solution was treated at 0° with 12.4 g. F<sub>2</sub>C<sub>1</sub>C<sub>6</sub>H<sub>4</sub>I, the mixture stirred 1 hr., refluxed 2 hrs., and worked up as before to yield 1 g. I. I was also prepared by adding 255 g. mixture of 45% hexafluorobenzene, 40% III, and 10% tetrafluorobenzene to 200 g. iodine in 1 kg. 65% oleum. The mixture was stirred 4 hrs. at 55-60°, let cool overnight, then in an ice bath, diluted with 2 l. ice H<sub>2</sub>O, decolorized with aqueous NaHSO<sub>3</sub>, and separated. The crude I (177 g.)

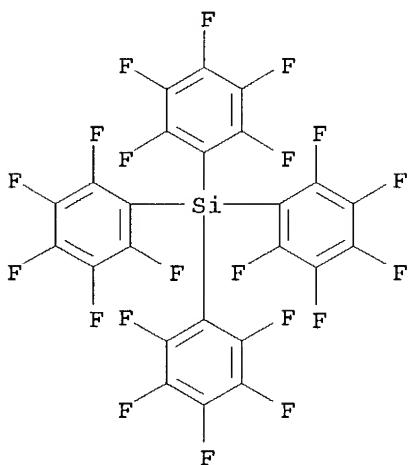
was

dried and distilled to give 36 g. I. Condensation of II in the presence of Cu powder at 180-90° 48 hrs. then at 290° 6 hrs. gave 87% (C<sub>6</sub>F<sub>5</sub>)<sub>2</sub>, sublimed at 50°/1 mm., m. 67.5-68°. I (5 g.) and 1.6 g. CuCN heated to 150° in 1.34 g. C<sub>5</sub>H<sub>5</sub>N, cooled to 100°, and distilled gave 3.07 g. crude C<sub>6</sub>F<sub>5</sub>CN (IV), b. 18590°, n<sub>D</sub> 23.8D 1.4764. Hydrolysis of IV with 75% H<sub>2</sub>SO<sub>4</sub> at 180° gave 16% C<sub>6</sub>F<sub>5</sub>CO<sub>2</sub>H, m. 101-3°. To the Grignard reagent from 10 g. II was added 6.6 g. AcH at 0°, the solution stirred 1 hr. at 0°, decomposed with 50 ml. 6N HCl, the Et<sub>2</sub>O layer separated, dried, and distilled to give 81% C<sub>6</sub>F<sub>5</sub>CHMeOH (V), b<sub>37</sub> 80-2°, n<sub>D</sub> 20D 1.4426. To the Grignard reagent from 24.7 g. II in 50 ml. Et<sub>2</sub>O was added 4.25 g. SiCl<sub>4</sub> at 0°, the mixture stirred 0.5 hr. at 0° refluxed 2.5 hrs., let cool overnight, poured into 100 ml. 6N HCl, and filtered. The solid was sublimed at 208°/1 mm. to give 32% (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Si, m. 246-8°. To the Grignard reagent from 30 g. II in 0.75 ml. Et<sub>2</sub>O was added 5.0 g. PCl<sub>3</sub> in 20 ml. Et<sub>2</sub>O in an ice bath, the mixture let stand at room temperature 15 min., hydrolyzed with 40 ml. cold 10% HCl, the Et<sub>2</sub>O layer separated, dried, and concentrated Sublimation at 100-30° under reduced pressure gave 39.5% (C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>P (VI), m. 114-15°. Oxidation of 2.0 g. VI by refluxing in 10 g. Na<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>, 25 ml. H<sub>2</sub>O, 10 ml. concentrated H<sub>2</sub>SO<sub>4</sub>, and 25 ml. AcOH gave, after neutralization and extraction with CHCl<sub>3</sub>, 2 g. (C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>PO, m. 167-8°. Pyrolysis of 2 g. V over Al<sub>2</sub>O<sub>3</sub> at 345-50° gave, after distillation, 0.6 g. C<sub>6</sub>F<sub>5</sub>CH: CH<sub>2</sub>, b. 140-1°, n<sub>D</sub> 20D 1.4414.

IT 1524-78-3, Silane, tetrakis(pentafluorophenyl) -  
(preparation of)

RN 1524-78-3 CAPLUS

CN Silane, tetrakis(pentafluorophenyl) - (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29 (Noncondensed Aromatic Compounds)

IT Benzene, tetrabromo-  
(manufacture of)

IT 608-71-9, Phenol, pentabromo-  
(manufacture of)

IT 87-82-1, Benzene, hexabromo- 108-72-5, 1,3,5-Benzenetriamine 434-90-2,  
 Biphenyl, decafluoro- 602-94-8, Benzoic acid, pentafluoro- 653-34-9,  
 Styrene, 2,3,4,5,6-pentafluoro- 773-82-0, Benzonitrile, pentafluoro-  
 827-15-6, Benzene, pentafluoroiodo- 830-50-2, Benzyl alcohol,  
 2,3,4,5,6-pentafluoro- $\alpha$ -methyl- 1259-35-4, Phosphine,  
 tris(pentafluorophenyl)- 1524-78-3, Silane,  
 tetrakis(pentafluorophenyl)- 2729-11-5, Phosphine oxide,  
 tris(pentafluorophenyl)- 13654-09-6, Biphenyl, decabromo- 27858-07-7,  
 Biphenyl, octabromo- 90823-46-4, Aniline, tetrabromo-  
 (preparation of)

L59 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:429701 CAPLUS

DOCUMENT NUMBER: 57:29701

ORIGINAL REFERENCE NO.: 57:5944a-h

TITLE: Synthesis of organosilicon compounds, particularly  
 those containing halophenyl groups

AUTHOR(S): Gilman, Henry; Gorsich, Richard D.; Gaj, Bernard J.

CORPORATE SOURCE: Iowa State Univ., Ames

SOURCE: Journal of Organic Chemistry (1962), 27, 1023-6  
 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. CA 55, 5416e. Tetrasubstituted silanes RnSiR'4-n (I) were prepared by treating RLi with the appropriate chlorosilane or SiCl4. Several compds., R3SiR'SiR3 (II) were prepared BuLi (0.05 mole) in 170 ml. Et2O stirred rapidly with gradual addition of 0.05 mole m-C6H4BrF in 95 ml. Et2O at -45°, the mixture stirred 20 min. at -40° and carbonated, the organic layer extracted with NaHCO3, the extract boiled and acidified with concentrated

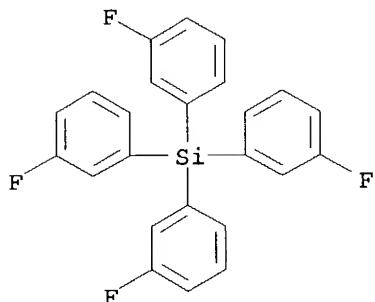
HCl yielded 65% m-FC6H4CO2H, m. 123-4°. Cl2SiPh2 (0.05 mole) in 80 ml. Et2O stirred with gradual addition of 0.12 mole m-FC6H4Li in 200 ml. Et2O and the mixture stirred 8 hrs. at 20°, refluxed 2 hrs. and the product taken up in ligroine (b. 60-70°), the solution decolorized (Norit) and evaporated yielded 26% I (R = m-FC6H4, R' = Ph, n = 2), m. 195-6°. Similarly were prepared I (R = m-FC6H4) (R', n, m.p. or b.p./mm., and % yield given): Ph, 1, 207-8° (AcOH), 51; Ph, 2, 195-6° (ligroine), 26; Ph, 3, 191.5-3.0° (dioxane), 51; 0, 4, 196-7° (ligroine), 62; C12H25, 3, 35-7°, 197 8°/0.02, n25D 1.5358, 62; C16H33, 8, 36-8°, 214-17°/0.05, 71; C18H37, 3, 38-40°, 234-5°/0.08, 71. GeCl4 (8.0 g.) and 0.178 mole m-FC6H4Li in 300 ml. Et2O yielded 25% (m-FC6H4)4Ge, m. 194-5° (ligroine). Similarly were prepared I using m-ClC6H4Li or p-ClC6H4Li (R, R', n, m.p. or b.p./mm., n25D, d25, MR, and % yield given): m-ClC6H4, Ph, 1, 156-7° (alc.), 78; m-ClC6H4, Ph, 2, 110-11° (alc.), 80; m-ClC6H4, Ph, 3, 87.5-9.0° (alc.), 43; m-ClC6H4, -, 4, 148-9° (ligroine), 43; m-ClC6H4, C12H25, 3, 229-30°/0.086 -, -, 78.5; m-ClC6H4, C16H33, 3, 240-1°/less than 0.01, 1.5579, 1.078, 175.9, 65.8; m-ClC6H4, C12H25, 3, 250-5°/0.04, 1.5595, 1.085, 183.5, 87.4; p-ClC6H4, C16H33, 3, 246-51°/0.03, 1.5530, 1.071, 175.7, 65.6; p-ClC6H4, C18H37, 3, 255-62°/0.001, 1.5558, 1.075, 183.4, 76.8. PhCH2MgCl

(25.3 g. PhCH<sub>2</sub>Cl, 4.86 g. Mg) in 200 ml. Et<sub>2</sub>O added with stirring to 5.9 g. Cl<sub>3</sub>SiCH<sub>2</sub>CH<sub>2</sub>SiCl<sub>3</sub> in 55 ml. Et<sub>2</sub>O and the mixture distilled 12 hrs., the Et<sub>2</sub>O replaced with xylene and refluxed 50 hrs. at 100°, hydrolyzed with 5% HCl and the product (11.6 g.) recrystd. 3 times from ligroine (b. 60-70°) and from EtOAc yielded 81% II [R = PhCH<sub>2</sub>, R' = (CH<sub>2</sub>)<sub>2</sub>], m. 136-7°. Similarly were prepared II (R, R', m.p. or b.p./mm., and % yield given): BuCH(Et)CH<sub>2</sub>, (CH<sub>2</sub>)<sub>2</sub>, 215-20°/0.04, 54; C<sub>16</sub>H<sub>33</sub>, (CH<sub>2</sub>)<sub>2</sub>, 43-5° (CCl<sub>4</sub>-alc.), 75; PhCH<sub>2</sub>, m-C<sub>6</sub>H<sub>4</sub>, 155-7° (EtOAc), 16; C<sub>10</sub>H<sub>21</sub>, m-C<sub>6</sub>H<sub>4</sub>, 285-8°/0.03, n<sub>20D</sub> 1.4811, d<sub>20</sub> 0.863, MR 323.8, 58; C<sub>10</sub>H<sub>21</sub>, p-C<sub>6</sub>H<sub>4</sub>, 290-4°/0.07, 20. Li (0.9 g.) in 60 ml. Et<sub>2</sub>O and 8.0 g. BrCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>:CH<sub>2</sub> in 70 ml. Et<sub>2</sub>O at -30° treated with 7.38 g. Ph<sub>3</sub>SiCl in 60 ml. Et<sub>2</sub>O and the mixture stirred 15 min. at 0° and 11 hrs. at 20°, hydrolyzed and the product distilled in vacuo gave material, b<sub>0.15</sub> 155-7°, recrystd. from alc. (ice bath) to yield 67% H<sub>2</sub>C:CH(CH<sub>2</sub>)<sub>3</sub>SiPh<sub>3</sub> (III), m. 45-6°. Ph<sub>3</sub>SiH (26 g.), 3.4 g. III, and 0.32 g. Bz<sub>2</sub>O<sub>2</sub> stirred 20 hrs. at 80° in 25 ml. C<sub>6</sub>H<sub>14</sub> and freed from excess Ph<sub>3</sub>SiH at 148-60°/0.7 mm., the gummy solid crystallized from alc. MeCOEt and the product, m. 140-3°, recrystd. from alc.-EtOAc yielded 65% pure II [R = Ph, R' = (CH<sub>2</sub>)<sub>5</sub>] (IV), m. 145-6°. Li(CH<sub>2</sub>)<sub>5</sub>Li (from 20 g. Br(CH<sub>2</sub>)<sub>5</sub>Br) in 180 ml. Et<sub>2</sub>O treated at -20° with 17.4 g. Ph<sub>3</sub>SiCl in 160 ml. Et<sub>2</sub>O and the mixture stirred 16 hrs. at 20°, hydrolyzed and the product crystallized from EtOAc gave IV. Et<sub>2</sub>O (30 ml.) containing 6 g. (3-BrC<sub>6</sub>H<sub>4</sub>)<sub>2</sub> added with stirring to 0.038 mole BuLi in 75 ml. Et<sub>2</sub>O at -30° and the mixture stirred 6 hrs. at 20°, refluxed 15 min. and the insol. reagent refluxed 45 min. with 11.3 g. Ph<sub>3</sub>SiCl in 100 ml. Et<sub>2</sub>O, diluted with 100 ml. C<sub>6</sub>H<sub>6</sub> and distilled to a pot temperature of 53°, refluxed 15 min. and hydrolyzed, the mixture filtered and the product recrystd. from H<sub>2</sub>O-dioxane yielded 69% II (R = Ph, R' = 3,3'-biphenylene), m. 221-3°.

IT 3869-53-2, Silane, tetrakis(m-fluorophenyl)-  
(preparation of)

RN 3869-53-2 CAPLUS

CN Silane, tetrakis(3-fluorophenyl)- (9CI) (CA INDEX NAME)



CC 33 (Organometallic and Organometalloidal Compounds)

IT 7803-62-5, Silane  
(halophenyl derivs.)

IT 2128-45-2, Silane, dodecyltris(m-fluorophenyl)- 2376-83-2, Silane,  
tris(m-fluorophenyl)hexadecyl- 2559-39-9, Silane, (m-

fluorophenyl)triphenyl- 2736-28-9, Silane, 4-pentenyltriphenyl-  
 2794-05-0, Silane, tris(m-fluorophenyl)octadecyl- 2804-88-8, Silane,  
 tris(m-fluorophenyl)phenyl- 2804-94-6, Silane, bis(m-  
 fluorophenyl)diphenyl- 3797-46-4, Germane, tetrakis(m-fluorophenyl)  
**3869-53-2**, Silane, tetrakis(m-fluorophenyl)- 18733-70-5, Silane,  
 bis(m-chlorophenyl)diphenyl- 18733-82-9, Silane, tetrakis(m-  
 chlorophenyl)- 18733-90-9, Silane, tris(m-chlorophenyl)phenyl-  
 18737-43-4, Silane, (m-chlorophenyl)triphenyl- 18759-06-3, Silane,  
 tris(m-chlorophenyl)hexadecyl- 18759-07-4, Silane, tris(p-  
 chlorophenyl)hexadecyl- 18764-96-0, Silane, tris(m-chlorophenyl)dodecyl-  
 18817-52-2, Silane, tris(m-chlorophenyl)octadecyl- 18817-86-2, Silane,  
 tris(p-chlorophenyl)octadecyl- 18826-15-8, Silane, 3,3'-  
 biphenylenebis[triphenyl- 18828-71-2, 2,5-Disilahexane,  
 2,2,5,5-tetrabenzyl-1,6-diphenyl- 18840-86-3, Silane,  
 m-phenylenebis[tribenzyl- 18846-53-2, 1,7-Disilaheptane,  
 1,1,1,7,7,7-hexaphenyl- 18863-01-9, Silane, m-phenylenebis[trisdecyl]-  
 18863-02-0, Silane, p-phenylenebis[tris(decyl)- 18867-29-3,  
 17,20-Disilahexatriacontane, 17,17,20,20-tetrahexadecyl- 18870-57-0,  
 Benzhydrol,  $\alpha$ -[(methyldiphenylsilyl)methyl]- 18882-14-9,  
 7,10-Disilahexadecane, 5,12-diethyl-7,7,10,10-tetrakis(2-ethylhexyl)-  
 (preparation of)

L59 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1961:93280 CAPLUS  
 DOCUMENT NUMBER: 55:93280  
 ORIGINAL REFERENCE NO.: 55:17557a-c  
 TITLE: Preparation and thermal stability of  
       tetrakis(pentafluorophenyl)silane and  
       tris(pentafluorophenyl)phosphine  
 AUTHOR(S): Wall, Leo A.; Donadio, Robert E.; Pummer, Walter J.  
 CORPORATE SOURCE: Natl. Bur. of Standards, Washington, DC  
 SOURCE: Journal of the American Chemical Society (1960), 82,  
       2846-8  
 CODEN: JACSAT; ISSN: 0002-7863

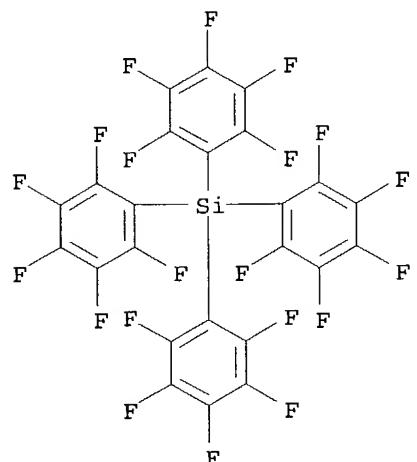
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB To C<sub>6</sub>F<sub>5</sub>MgBr (from 24.7 g. C<sub>6</sub>F<sub>5</sub>Br, 2.43 g. Mg and 50 ml. dry Et<sub>2</sub>O) was added dropwise 4.25 g. SiCl<sub>4</sub> at 0°, the whole stirred 1 hr. at 0° and refluxed 3 hrs. to give 32% (C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>Si (I), m. 248-50° (sublimation at 208°/1 mm. followed by recrystn. from Me<sub>2</sub>CO-C<sub>6</sub>H<sub>6</sub>),  $\lambda$  6.57, 7.72, 9.1, 10.26  $\mu$ . Attempts to prepare (C<sub>6</sub>F<sub>5</sub>)<sub>2</sub>SiCl<sub>2</sub> by this procedure gave some I and tars. The same procedure gave 39.5% (C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>P (II), m. 116-17°,  $\lambda$  6.08, 6.57, 6.78, 10.25  $\mu$ ,  $\lambda$ MeOHmax. 253  $\text{m}\mu$  ( $\epsilon$  = 10,400). II (2.0 g.), 10 g. Na<sub>2</sub>CrO<sub>7</sub>, 25 ml. H<sub>2</sub>O, 10 ml. concentrated H<sub>2</sub>SO<sub>4</sub>, and 25 ml. AcOH refluxed 6 hrs. gave 2.0 g. (C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>PO (III), m. 169-70° (petr. ether),  $\lambda$  6.08, 6.59, 6.75, 8.15, 10.15  $\mu$ ;  $\lambda$ MeOHmax. 2.75, 250  $\text{m}\mu$  ( $\epsilon$  = 2600, 730). The thermal stability of I, II, III, Ph<sub>2</sub> (IV), (C<sub>6</sub>F<sub>5</sub>)<sub>2</sub> (V), Ph<sub>4</sub>Si (VI), and Ph<sub>3</sub>P (VII) at 200-660° indicated the following order: V ≥ IV > VI ≥ I > II > VII > III.

IT **1524-78-3**, Silane, tetrakis(pentafluorophenyl)-  
 (preparation and thermal stability of)

RN 1524-78-3 CAPLUS  
CN Silane, tetrakis(pentafluorophenyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 10E (Organic Chemistry: Benzene Derivatives)  
IT Phosphine, diphenylpiperidino-  
IT 1259-35-4, Phosphine, tris(pentafluorophenyl)- 1524-78-3,  
Silane, tetrakis(pentafluorophenyl)- 2729-11-5, Phosphine oxide,  
tris(pentafluorophenyl)-  
(preparation and thermal stability of)  
IT 35259-94-0, Phosphine sulfide, diphenylpiperidino-  
(preparation of)  
IT 92-52-4, Biphenyl 434-90-2, Biphenyl, decafluoro- 603-35-0, Phosphine,  
triphenyl- 1048-08-4, Silane, tetraphenyl-  
(thermal stability of)

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